PREDICTING CERIUM + H_2O CLUSTER FORMATION WITH SIMULATED AND EXPERIMENTAL SPECTROSCOPY

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Ceria (CeO_2) has been established as a good support in heterogeneous catalysts for the water gas shift reaction. This study looks into cerium's reactivity with water, a water gas shift reagent, and aims to build an understanding of the three reactions which can occur: direct oxidation, -OH abstraction, and H_2O addition. Through the use of anion photoelectron spectroscopy and density functional theory calculations we have been able to determine that the reactivity is dependent on (1) the oxidation states of the metal centers, (2) the availability of 5d orbitals to form metal oxide bonds, and (3) the presence of electrons in the 6s* orbital. The results of this study can be used to inform design of catalytic materials for the water gas shift reaction.